We Claim:

1. A crystallized acyl carrier protein synthase (ACPS) enzyme.

2. The crystallized ACPS enzyme of Claim 1, wherein said ACPS enzyme comprises amino acid residues ASP8, GLU11, ARG14, MET18, PHE25, ARG28, ILE29, ARG45, PHE49, ARG53, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68, PHE74, LYS81, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105, or conservative substitutions thereof.

3. The crystallized ACPS enzyme of Claim 1, wherein said ACPS enzyme comprises amino acid residues ASP8, PHE25, ARG28, ILE29, ARG53, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68, PHE74, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105, or conservative substitutions thereof.

4. The crystallized ACPS enzyme of Claim 1, wherein said ACPS enzyme comprises amino acid residues ILE5, GLY6, LEU7, ILE9, THR10, ARG14, ILE15, MET18, GLN22, LEU41, ARG45, GLU48, PHE49, LEU50, ALA51, GLY52, ALA55, LYS57, ALA59, PHE60, ALA63, PHE64, GLY69, ARG70, GLN71, LEU72, ILE79, ARG80, LYS81, ASP82, GLN83, TYR88, VAL101, SER102, THR106, TYR109, ALA110, and ALA111, or conservative substitutions thereof.

5. The crystallized ACPS enzyme of Claim 1, wherein said ACPS enzyme comprises amino acid residues GLY6, ASP8, ALA51, ARG53, LYS57, GLU58, ALA59, LYS62, and ALA63, or conservative substitutions thereof.

6. The crystallized ACPS enzyme of Claim 1, characterized as being in plate form with space group $P2_1$, and having unit cell parameters of a=76.26Å, b=76.16Å, c=85.69 Å, and beta=93.3°.

7. The crystallized ACPS enzyme of Claim 6, further characterized as consisting of six molecules of ACPS in an asymmetric unit.

8. A crystallized complex comprising acyl carrier protein synthase (ACPS) and coenzyme A (CoA).

9. The crystallized complex of Claim 8, wherein the ACPS enzyme comprises amino acid residues ASP8, GLU11, ARG14, MET18, PHE25, ARG28, ILE29, ARG45, PHE49, ARG53, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68, PHE74, LYS81, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105, or conservative substitutions thereof.

10. The crystallized complex of Claim 8, wherein the ACPS comprises amino acid residues ASP8, PHE25, ARG28, ILE29, ARG53, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68, PHE74, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105, or conservative substitutions thereof.

11. The crystallized complex of Claim 8, wherein the ACPS comprises amino acid residues ILE5, GLY6, LEU7, ILE9, THR10, ARG14, ILE15, MET18, GLN22, LEU41, ARG45, GLU48, PHE49, LEU50, ALA51, GLY52, ALA55, LYS57, ALA59, PHE60, ALA63, PHE64, GLY69, ARG70, GLN71, LEU72, ILE79, ARG80, LYS81, ASP82, GLN83, TYR88, VAL101, SER102, THR106, TYR109, ALA110, and ALA111, or conservative substitutions thereof.

12. The crystallized complex of Claim 8, wherein the ACPS comprises amino acid residues GLY6, ASP8, ALA51, ARG53, LYS57, GLU58, ALA59, LYS62, and ALA63, or conservative substitutions thereof.

13. The crystallized complex of Claim 8, characterized as being in pyramidal form with space group R3, and having unit cell parameters of a=b=55.82Å and c=92.28Å.

14. The crystallized complex of Claim 13, further characterized as consisting of one molecule of ACPS and one molecule of CoA in an asymmetric unit.

15. A method for identifying an agent that interacts with an active site of ACPS, comprising the steps of:

(a) determining an active site of ACPS from a three dimensional model of the ACPS enzyme; and

(b) performing computer fitting analysis to identify an agent which interacts with said active site.

16. The method of Claim 15, further comprising contacting the identified agent with ACPS in order to determine the effect the agent has on ACPS activity.

17. The method of Claim 16, wherein the agent is an inhibitor of ACPS activity.

18. The method of Claim 16, wherein the agent is an activator of ACPS activity.

19. A method for identifying an agent that interacts with an active site of ACPS-CoA complex comprising the steps of:

(a) determining an active site of the ACPS-CoA complex from a three dimensional model of the ACPS-CoA complex; and

(b) performing computer fitting analysis to identify an agent which interacts with said active site.

20. The method of Claim 19, further comprising contacting the identified agent with ACPS-CoA complex in order to determine the effect the agent has on ACPS-CoA complex activity.

21. The method of Claim 20, wherein the agent is an inhibitor of ACPS-CoA complex activity.

22. The method of Claim 21, wherein the agent is an activator of ACPS-CoA complex activity.

23. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising a CoA binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or molecular complex comprising a CoA binding site using the relative structural coordinates according to Figure 1 or 2 of residues ARG45, PHE49, ARG53, LYS81, ASN84, GLY85, LYS86, PRO87, ILE103, THR104 and HIS105 from one monomer of ACPS, and ASP8, GLU11, ARG14, MET18, PHE25, ARG28, ILE29, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68 and PHE74 from a second monomer of ACPS, in each case ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

(b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis with the three dimensional model generated in step (a);

(c) obtaining the candidate activator or inhibitor; and

(d) contacting the candidate activator or inhibitor with said molecule or molecular complex and measuring the effect the candidate activator or inhibitor has on said molecule or molecular complex.

24. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising a CoA binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or molecular complex comprising a CoA binding site using the relative structural coordinates according to Figure 1 or 2 of residues ARG53, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105 from one monomer of ACPS and residues ASP8, PHE25, ARG28, ILE29, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68 and PHE74 from a second monomer of ACPS, in each case ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

(b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis with the three dimensional model generated in step (a);

(c) obtaining the candidate activator or inhibitor; and

(d) contacting the candidate activator or inhibitor with said molecule or molecular complex and measuring the effect the candidate activator or inhibitor has on said molecule or molecular complex.

25. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising a CoA binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or molecular complex comprising a CoA binding site using the relative structural coordinates according to Figure 1 or 2 of residues LEU41, ARG45, GLU48, PHE49, LEU50, ALA51, GLY52, ILE79, ARG80, LYS81, ASP82, GLN83, TYR88, VAL101, SER102, THR106, TYR109, ALA110, and ALA111 from one monomer of ACPS and residues ILE5, GLY6, LEU7, ILE9, THR10, ARG14, ILE15, MET18, GLN22, ALA55, LYS57, ALA59, PHE60, ALA63, PHE64, GLY69, ARG70, GLN71 and LEU72 from a second monomer of ACPS, in each case ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

(b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis with the three dimensional model generated in step (a);

(c) obtaining the candidate activator or inhibitor; and

(d) contacting the candidate activator or inhibitor with said molecule or molecular complex and measuring the effect the candidate activator or inhibitor has on said molecule or molecular complex.

26. An agent identified by the method of Claim 23.

27. An agent identified by the method of Claim 24.

28. An agent identified by the method of Claim 25.

29. A method for determining the molecular structure of a molecule or molecular complex whose structure is unknown, comprising the steps of:

(a) obtaining crystals of the molecule or molecular complex whose structure is unknown;

(b) generating X-ray diffraction data from the crystallized molecule or molecular complex;

(c) comparing the X-ray diffraction data from the molecule or molecular complex with the three dimensional structure determined from the crystal of Claim 1; and

(d) using molecular replacement analysis to conform the three dimensional structure determined from the crystal of Claim 1 to the X-ray diffraction data from the crystallized molecule or molecular complex.

30. A method of determining the molecular structure of a molecule or molecular complex whose structure is unknown, comprising the steps of:

(a) obtaining crystals of the molecule or molecular complex whose structure is unknown;

(b) generating X-ray diffraction data from the crystallized molecule or molecular complex;

(c) comparing the X-ray diffraction data from the molecule or molecular complex with the three dimensional structure determined from the crystal complex of Claim 7; and

(d) using molecular replacement analysis to conform the three dimensional structure determined from the crystal complex of Claim 7 to the X-ray diffraction data from the crystallized molecule or molecular complex.

31. An active site of an acyl carrier protein synthase comprising the structural coordinates according to Figure 1 or 2 of residues ARG45, PHE49, ARG53, LYS81, ASN84, GLY85, LYS86, PRO87, ILE103, THR104 and HIS105 from one monomer of ACPS, and of ASP8, GLU11, ARG14, MET18, PHE25, ARG28, ILE29, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68 and PHE74

from a second monomer of ACPS, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

32. An active site of an acyl carrier protein synthase comprising the structural coordinates according to Figure 1 or 2 of residues ARG53, ASN84, GLY85, LYS86, PRO87, ILE103, THR104, and HIS105 from one monomer of ACPS and of residues ASP8, PHE25, ARG28, ILE29, PHE54, GLU58, SER61, LYS62, GLY65, THR66, GLY67, ILE68 and PHE74 from a second monomer of ACPS, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

33. An active site of an acyl carrier protein synthase comprising the structural coordinates according to Figure 1 or 2 of residues LEU41, ARG45, GLU48, PHE49, LEU50, ALA51, GLY52, ILE79, ARG80, LYS81, ASP82, GLN83, TYR88, VAL101, SER102, THR106, TYR109, ALA110, and ALA111 from one monomer of ACPS and of residues ILE5, GLY6, LEU7, ILE9, THR10, ARG14, ILE15, MET18, GLN22, ALA55, LYS57, ALA59, PHE60, ALA63, PHE64, GLY69, ARG70, GLN71 and LEU72 from a second monomer of ACPS, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

34. An active site of an acyl carrier protein synthase comprising the structural coordinates of GLY6, ASP8, ALA51, ARG53, LYS57, GLU58, ALA59, LYS62, and ALA63 according to Figure 1 or 2, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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